Cross-Cutting Topics

Carbon Capture Workshop – October 5-6, 2009

Crosscutting Topics

Approaches
- Combinations of technologies
- Chemical looping
- Setting targets vs. standards
- Alternative regeneration schemes

Assessment (iterative)

Issues
- Water management
- CO_2 compression
- Sequestration specs
- Contaminants
- Technology deployment planning
- Scale up
  - Ability to predict attrition of solids (e.g., sorbants, oxidants, reactants, ash)
- Environmental footprint

Methodologies
- Holistic modeling
- Computation/numerical simulation
- Characterization tools
- Sensor & controls
- Standards for comparison

Interaction Between Capture & Sequestration
- Purity of CO_2
- Pressure specs
- Intermittency

Oxy-Fuels

TRL: Pilots

Challenges (moving up):

- Corrosion on fire side; new materials
- Air in-leakage contaminants (e.g. N_2 and argon) and how to remove cost effectively
- Boiler design improvements
- Understand how to deal with complexity ("plumbing problems" and process optimization)
  - Reliability, Sizing, Transients
  - Approach: 1) Learn from existing demos; 2) dynamic simulation development and validation; 3) learn from risk/availability assessments

Challenge (in between):

- Radiation model with validation (Is it significant?)

Challenges (moving down):

- Capital and operating cost reduction breakthrough in oxygen separation (beyond most advanced of today)
- Basic separations research
- Boiler design fundamental understanding
- Materials of construction
- Particle reactions under oxy-fuel conditions

Chemical Looping

TRL: Pilots to Engineering Science

Challenges (moving up):
- Lifecycle and environmental impact of oxidants
- How to implement retrofits
- Transport/solids management
- Heat management/new reactor concepts
- Sensor & controls (pilots)
- Sorbant reclamation and ash management

Challenges (moving down):
- Approaches for dealing with contaminants
- Understanding mechanism for reactions between two solid materials
- Durability of oxidants
- How to get more balanced thermodynamics
  - New processes
  - Fundamental physics of particles
  - New chemistry materials (e.g., nanostructured materials)
  - New compostitions
  - New construction materials (to combat erosion)

Computation and Characterization
(Multi-scale Physics)

TRL: Across all TRLs

Challenges:

- Lack of particle scale information needed as inputs to macro-scale models
- Lack of understanding of mechanisms for capture (e.g., diffusion or adsorption in case of solid adsorbents
- Getting enough information from bench work to do economic analysis
- Developing fundamental understanding that will lead to scale-bridging models/reduced order models
- Developing scale-bridging models/reduced order models
- Improved numerical methods
- Model validation across spectrum of scales (particle, bench, pilot, commercial)
- Uncertainty quantification (e.g., inputs, boundary, external validation, data, etc.)
- Developing virtual models (to help minimize “plumbing problems”)
- Better data and understanding of speciation and fate of trace elements
- Improve modeling of weak interactions for materials discovery

CO_2 Compression

TRL: System engineering (across multiple technologies)

Challenges (moving up):

- Systems study to reconcile commercial equipment supply with theoretical specs.
- Understanding different compression needs as function of technical approach to capture (e.g., membranes, absorbents, etc.)
- Understand issues with scaling up GPUs
- Lack of pilot plant data collection of gas composition and contaminants
- Lack of pilot plant data collection of condensate (water) composition

Challenges (moving down):

- Fundamental understanding of CO_2 physical properties in presence of contaminants (e.g., water and acid gas) and also solubility in brine
- Lack of transport models to understand pressure specs for output CO_2
- Materials corrosion/compatibility issues

Alternatives to Sequestration
(CO_2 as Feedstock)

TRL: Basic science

Challenges:

- What are options? Fundamental scientific inquiry into options
- Determine ways to independently tune thermodynamics and kinetics of any CO_2 reaction
- Investigate chemistry that is separate from acid-based chemistry)
- Investigate biological approaches
- Chemistry needs to scale with the problem
  - Mineralization, building materials, fuel, chemicals*

***** *Higher value chemicals may be pathway to innovation, but they are not solution*

Speciation and Fate of Trace Elements

TRL: Across all TRLs

Challenges

- Modeling
- What are mechanisms?
- Experimental measurements
- Sensing and detection
- Quantifying environmental impact
- Impact on carbon capture

Scale Up and Technology Development

TRL: Across all TRLs

Challenges

- Can high performance computing/modeling/simulation be used to accelerate scale up?
- What algorithms are needed?
- Can we find a better way to integrate tools?
- How can we remedy lack of computer access, lack of funding?
- How do we use computations to develop better models and necessary data?
- What are gaps in capabilities from the user's perspective?
- Can we catalogue where modeling is used today for scale up?

Note: Perhaps more of an FE pull than a SC push

Alternative Regeneration Schemes

TRL: Across lower half of TRLs

Challenges

• Develop Co2 release processes with more efficiency than temperature/pressure swing

- Chemical reactions (reduction)
- Electrolytic stripping
- Mineralization
- Phase change

• Develop standard comparison of energy consumption and cost

New Agenda Item: Communication

DOE needs to develop mechanisms to facilitate dialogue and knowledge sharing up and down the TRL ladder. Find ways to build a broader and more cohesive carbon capture community, including sub-communities. Example: Sandia combustion labs (partially due to physical proximity)

Possible drivers:

- Additional funding
- Focused conferences
- Invited publications
- Make a dissemination plan a requirement
- Communicate lessons-learned “down the ladder”
- Funding structured to promote project manager “matchmaking” between basic and applied R&D teams
- Grad student fellowships/internships
- Encourage links between basic and applied w/o discourageing “discovery” R&D by basic
- Need mechanism for “plucking out” basic science ideas for move to applied side